Unsupervised learning

Unsupervised learning

- in *supervised learning* we deal with pairs of records u, v
- goal is to predict v from u using a prediction model
- the output records v^i 'supervise' the learning of the model

- in *unsupervised learning*, we deal with only records u
- goal is to *build a data model* of u, in order to
  - *reveal structure* in u
  - *impute missing entries* (fields) in u
  - *detect anomalies*
- yes, the first goal is vague . . .

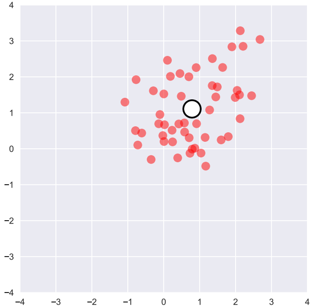
Embedding

- as usual we embed raw data u into a feature vector $x = \phi(u) \in \mathbf{R}^d$
- we then build a data model for the feature vectors
- we un-embed when needed, to go back to the raw vector u
- so we'll work with feature vectors from now on
- (embedded) data set has the form $x^1, \ldots, x^n \in \mathbf{R}^d$

Data model via loss function

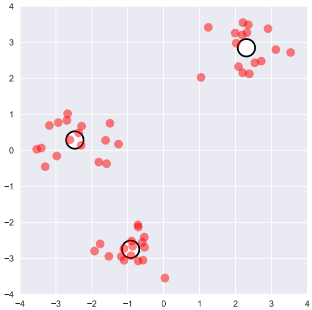
- a *data model* tells us what the vectors in some data set 'look like'
- can be expressed quantitatively by an *implausibility function* or *loss function* $\ell : \mathbf{R}^d \to \mathbf{R}$
- $\ell(x)$ is how implausible x is as a data point
  - $\ell(x)$ small means x 'looks like' our data, or is 'typical'
  - $\ell(x)$ large means x does not look like our data
- if our model is probabilistic, *i.e.*, x comes from a density $p(x)$, we can take $\ell(x) = -\log p(x)$, the *negative log density*
- other names for $\ell(x)$: surprise, perplexity, ...
- ℓ is often *parametrized* by a vector or matrix θ, and denoted $\ell_\theta(x)$

A simple constant model



- data model: *x is near a fixed vector $\theta \in \mathbf{R}^d$*
- $\theta \in \mathbf{R}^d$ parametrizes the model
- some implausibility functions:
  - $\ell_\theta(x) = ||x - \theta||_2^2 = \sum_{i=1}^d (x_i - \theta_i)^2$ (square loss)
  - $\ell_\theta(x) = ||x - \theta||_1 = \sum_{i=1}^d |x_i - \theta_i|$ (absolute loss)

k-means data model



- data model: *x is close to one of the k representatives $\theta_1, \ldots, \theta_k \in \mathbf{R}^d$*
- quantitatively: for our data points x, the quantity

$$\ell_\theta(x) = \min_{i=1,\ldots,k} ||x - \theta_i||_2^2$$

i.e., the minimum distance squared to the representatives, is small

- $d \times k$ matrix $\theta = [\theta_1 \cdots \theta_k]$ parametrizes the k-means data model

Role of loss function in supervised and unsupervised learning

- in supervised learning
  - a loss function is used to choose a particular predictor from a parameterized family of predictors
  - once we've chosen and validated our predictor, we don't care about the loss function
- in unsupervised learning
  - a loss function characterizes what the data looks like
  - the loss function is our data model, and is itself our primary goal

Anomaly detector

- a data model allows us to identify *suspicious* or *anomalous* feature vectors
- first choose or fit a data model, with loss function ℓ
- find the 99th (say) percentile t of $\ell(x^i)$ on some test data
- flag a feature vector x as anomalous if $\ell(x) > t$

Imputing missing entries

Imputing missing entries

- suppose x has some entries missing, denoted *?* or *NA* or *NaN*
- $\mathcal{K} \subseteq \{1, \ldots, d\}$ is the set of *known entries*
- we use our data model to guess or *impute* the missing entries
- we'll denote the imputed vector as $\hat{x}$
- $\hat{x}_i = x_i$ for $i \in \mathcal{K}$
- imputation example, with $\mathcal{K} = \{1, 3\}$

$$x = \begin{bmatrix} 12.1 \\ ? \\ -2.3 \\ ? \end{bmatrix} \qquad \Longrightarrow \qquad \hat{x} = \begin{bmatrix} 12.1 \\ -1.5 \\ -2.3 \\ 3.4 \end{bmatrix}$$

  - we are imputing or guessing $\hat{x}_2 = -1.5$, $\hat{x}_4 = 3.4$
  - the other entries we know: $\hat{x}_1 = x_1 = 12.1$, $\hat{x}_3 = x_3 = -2.3$

Application: Recommendation system

- features are movies; examples are customer ratings or *?* if the customer has not rated that movie
- imputed entries are our guess of *what rating the customer would give, if they rated that movie*
- we *recommend* movies to a customer
  - that they have not rated
  - and for which the imputed rating is large

Application: Filling in missing features for supervised learning

- setting: data set in supervised learning problem contains some missing features
- common approach: ignore any record that has any feature missing
- in some cases, you'll lose much of your data (and therefore do poorly at fitting a prediction model)
- alternative approach:
  - use imputation to fill in (presumably few) missing feature entries
  - then proceed with supervised learning

Application: Detecting anomalous entries

- goal is to flag suspicious or anomalous *entries* in x
- method based on imputation: for each i
  - pretend entry x_i in x is *?*
  - find its imputed value $\hat{x}_i$ (based on all other entries of x)
  - if x_i and $\hat{x}_i$ are very different, flag x_i as anomalous

Supervised learning as special case of imputation

- suppose we wish to predict $y \in \mathbf{R}^m$ based on $x \in \mathbf{R}^d$
- we have some training data $x^1, \ldots, x^n$, $y^1, \ldots, y^n$
- define $(d+m)$-vector $\tilde{x} = (x, y)$
- build data model for $\tilde{x}$ using training data $\tilde{x}^1, \ldots, \tilde{x}^n$
- to predict y given x, impute last m entries of $\tilde{x} = (x, ?)$

Imputation using a data model

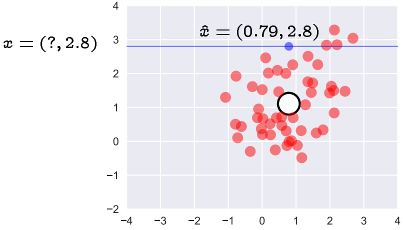
- given partially specified vector x we minimize over the unknown entries:

$$\begin{array}{ll} \text{minimize} & \ell_\theta(\hat{x}) \\ \text{subject to} & \hat{x}_i = x_i, \quad i \in \mathcal{K} \end{array}$$

- *i.e.*, impute the unknown entries to minimize the implausibility, subject to the given known entries

- . . . a simple and natural method

Imputing with constant data model



- given x with some entries unknown
- constant data model with implausibility function $\ell_\theta(x) = ||x - \theta||_2^2$
- we minimize $(\hat{x}_1 - \theta_1)^2 + \cdots + (\hat{x}_d - \theta_d)^2$ subject to $\hat{x}_i = x_i$ for $i \in \mathcal{K}$
- so $\hat{x}_i = x_i$ for $i \in \mathcal{K}$
- for $i \notin \mathcal{K}$, we take $\hat{x}_i = \theta_i$
- *i.e.*, for the unknown entries, guess the model parameter entries
- example has $\theta = (0.79, 1.11)$

Imputing with k-means data model

- given x with some entries unknown
- k-means data model with implausibility function $\ell_\theta(x) = \min_{i=1,\ldots,k} ||x - \theta_i||_2^2$
- find nearest representative θ_j to x, using only known entries
- *i.e.*, find j that minimizes $\sum_{i \in \mathcal{K}} (x_i - (\theta_j)_i)^2$
- guess $\hat{x}_i = (\theta_j)_i$ for $i \notin \mathcal{K}$
- *i.e.*, for the unknown entries, guess the entries of the closest representative

Validating imputation

we can validate a proposed data model (and imputation method):

- divide data into a training and a test set
- build data model on the training set
- mask some entries in the vectors in the test set (*i.e.*, replace them with *?*)
- impute these entries and evaluate the average error of the imputed values, *e.g.*, the RMSE

Fitting data models

Generic fitting method

- given data $x^1, \ldots, x^n$ (with no missing entries), and parametrized implausibility function $\ell_\theta(x)$
- how do we choose the parameter θ?

- average implausibility or *empirical loss* is

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell_\theta(x^i)$$

- choose θ to minimize $\mathcal{L}(\theta)$, (possibly) subject to $\theta \in \Theta$, the set of acceptable parameters
- *i.e.*, choose parameter θ so the observed data is least implausible

Fitting a constant model with sum squares loss

- sum squares implausibility function $\ell_\theta(x) = ||x - \theta||^2$
- empirical loss is

$$\mathcal{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} ||x^i - \theta||_2^2$$

- minimizing over θ yields

$$\theta = \frac{1}{n}\sum_{i=1}^{n} x^i$$

  the mean of the data vectors

Fitting a constant model with sum absolute loss

- sum absolute implausibility function $\ell_\theta(x) = ||x - \theta||_1$
- empirical loss is
$$\mathcal{L}(\theta) = \frac{1}{n}\sum_{i=1}^{n} ||x^i - \theta||_1$$
- minimizing over θ yields
$$\theta = \text{median}(x^1, \ldots, x^n)$$
the elementwise median of the data vectors

Fitting a k-means model

- implausibility function $\ell_\theta(x) = \min_{j=1,\ldots,k} ||x - \theta_j||^2$
- parameter is $d \times k$ matrix with columns $\theta_1, \ldots, \theta_k$
- empirical loss is

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \min_{j=1,\ldots,k} ||x^i - \theta_j||^2$$

- this is the k-means objective function!
- we can use the k-means algorithm to (approximately) minimize $\mathcal{L}(\theta)$, *i.e.*, fit a k-means model

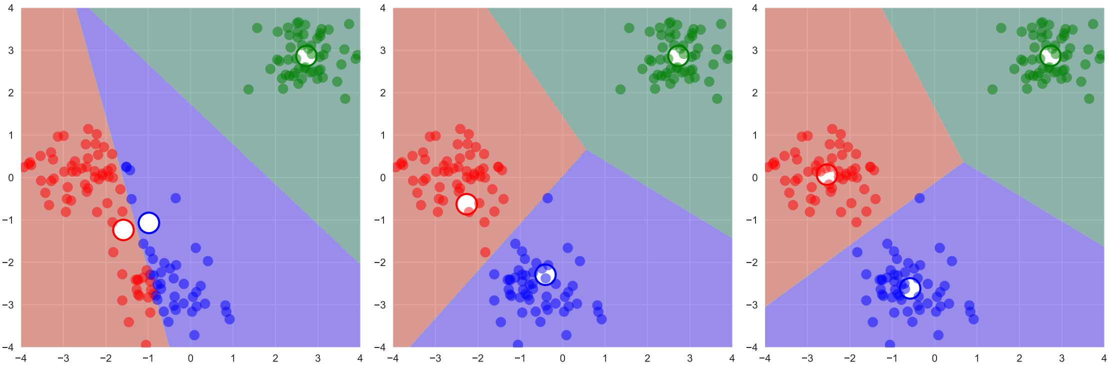
k-means algorithm

- define the *assignment* or *clustering* vector $c \in \mathbf{R}^n$
- c_i is the cluster that data vector x^i is in (so $c_i \in \{1, \ldots, k\}$)
- to minimize

$$\mathcal{L}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \min_{j=1,\ldots,k} ||x^i - \theta_j||^2$$

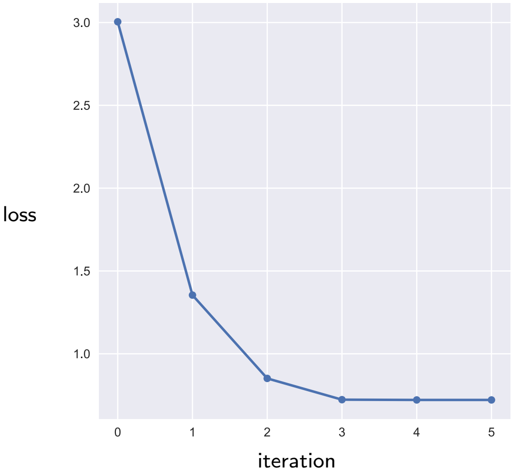
  we minimize $\frac{1}{n} \sum_{i=1}^{n} ||x^i - \theta_{c_i}||^2$ over both c and $\theta_1, \ldots, \theta_k$
- we can minimize over c using $c_i = \operatorname{argmin}_j ||x^i - \theta_j||^2$
- we can minimize over $\theta_1, \ldots, \theta_k$ using θ_i as the average of $\{x^j \mid c_j = i\}$
- k-means algorithm alternates between these two steps
- it is a heuristic for (approximately) minimizing $\mathcal{L}(\theta)$

k-means example



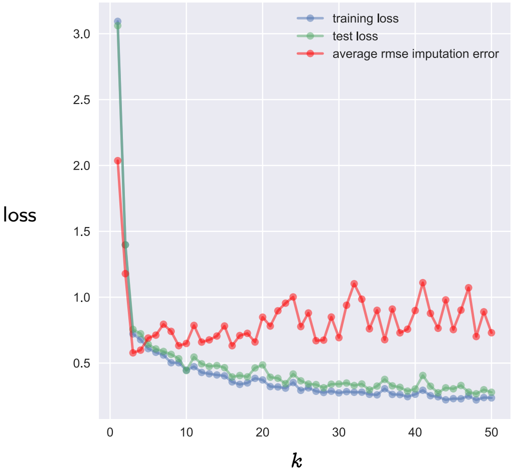
- 200 data points; reserve 40 for test

k-means example



- convergence after 4 iterations

k-means example



- fit k-mean data model for $k = 1, 2, \ldots, 50$
- validate by removing randomly either u_1 or u_2 from each record in test set